Boundary terms and their Hamiltonian dynamics

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It is described how the standard Poisson bracket formulas should be modified in order to incorporate integrals of divergences into the Hamiltonian formalism and why this is necessary. Examples from Einstein gravity and Yang-Mills gauge field theory are given.

1. INTRODUCTION

Hamiltonian mechanics traditionally serves as an étalon part of the mathematical physics both for physicists and mathematicians [1,2]. Many of its geometrical constructions are exported now to the field theory. For example, the Schouten-Nijenhuis bracket [3] turned out to be extremely useful in the search for integrable models during the last 20 years. In the pioneering article [4] this approach had been called as the formal variational calculus because in proving theorems it was possible to replace functionals by functions, even polynomials. Presently there are some monographs available where the method is presented comprehensively [5,6].

The main restriction required by this approach is the freedom to integrate by parts. This requirement is fulfilled if the fields are rapidly decaying at spatial infinity (as the massive fields usually do) or if the periodic boundary conditions are imposed. However, these cases do not cover all types of the physically interesting boundary behaviour. Often one has to deal with a slow decay of the gauge or gravitational fields at spatial infinity [7,8], with nonperiodical boundary conditions for a media moving in a finite domain [9] or for integrable models [10–12]. Can we still use the Hamiltonian approach in such cases? Of course, the answer is positive and the cited papers just do that. What we are trying to do here is to propose a more general framework for the nontrivial boundary problems.

In this report we intend to show that the main geometrical concepts of the formal variational calculus, and, consequently, the Hamiltonian mechanics, can be preserved without the standard requirement on the freedom to integrate by parts. In other words we propose an approach that does not neglect surface integrals. This purpose can be achieved by introduction of a new grading into the formal variational calculus [13] and a new pairing compatible with this grading. First of all, the revision consists in the modification of formulas for the Poisson bracket in field theory [14].

2. THE POISSON BRACKET

Briefly then, we will modify the standard formula for the Poisson bracket by surface terms in such a way that all its general axiomatic properties (bilinearity, antisymmetry, Jacobi identity and closeness, i.e., the requirement to remain in a given space of functionals) [5] will be preserved without discarding any term in the course of integration by parts.

Being one of the main elements of the Hamiltonian formalism the Poisson bracket itself is not elementary and may be considered as a composite structure

$$\{F,G\} = \mathsf{d}G \,\lrcorner\, \mathsf{d}F \,\lrcorner\, \Psi. \tag{1}$$

Its elements are: the differentials of functionals $\mathsf{d}F$, $\mathsf{d}G$, the Poisson bivector Ψ and the pairing (or interior product) operation $\lrcorner$. It turns out that in order to take care of all surface integrals we should revise all the three constituents of the bracket.

There are two ways to write a local functional: as an integral of some smooth function $\phi_A^{(J)}(x)$

of the fields and their spatial derivatives up to some finite order over the prescribed domain Ω in $\mathbb{R}^n$, or as the integral over all the space $\mathbb{R}^n$ but with the characteristic function of the domain θ_Ω included into the integrand

$$F = \int_\Omega f\left(\phi_A^{(J)}(x)\right) = \int \theta_\Omega f. \tag{2}$$

Henceforth we will consider the space $\mathbb{R}^n$, use the Einstein rule for summations and the multi-index notations $J = (j_1, ..., j_n)$ where $j_i \geq 0$

$$\phi_A^{(J)} = \frac{\partial^{|J|}\phi_A}{\partial^{j_1}x^1 ... \partial^{j_n}x^n}, \qquad |J| = j_1 + ... + j_n. \tag{3}$$

The reader unfamiliar with these notations may first have in mind the one-dimensional case, then J simply is the order of spatial coordinate derivative. Binomial coefficients for multi-indices are

$$\binom{J}{K} = \binom{j_1}{k_1} \cdots \binom{j_n}{k_n}, \tag{4}$$

$$\binom{j}{k} = \begin{cases} j!/(k!(j-k)!) & \text{if } 0 \leq k \leq j; \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

With the help of them we introduce the so-called higher Eulerian operators [15,16,5]

$$E_A^J(f) = (-1)^{|K|+|J|} \binom{K}{J} D_{K-J} \frac{\partial f}{\partial \phi_A^{(K)}}, \tag{6}$$

where

$$D_i = \frac{\partial}{\partial x^i} + \phi_A^{(J+i)} \frac{\partial}{\partial \phi_A^{(J)}}, \qquad D_J = D_1^{j_1} ... D_n^{j_n}. \tag{7}$$

In the framework of the standard approach the differential of a local functional is given by the Euler-Lagrange derivative $E_A^0(f)$

$$\mathsf{d}F = \int_\Omega E_A^0(f) \delta\phi_A. \tag{8}$$

This is fully justified if all variations $\delta\phi_A$ and all their spatial derivatives are zero on the boundary. In a more general case $E_A^0(f)$ gives us only a part of the full variation. As a consequence of that fact Euler-Lagrange derivatives may not commute [17]. In turn this leads us to the conclusion [18] that transformations of the form

$$q^A(x) \to q^A(x), \quad p_A(x) \to p_A(x) + \frac{\delta F[q]}{\delta q^A(x)}, \tag{9}$$

are, generally speaking, canonical only up to surface terms. Finally, as the standard proof of the Jacobi identity in mechanics is based on the commutativity of the mixed second derivatives, in field theory the Jacobi identity for functionals may not be true even if the fields themselves have the canonical Poisson brackets.

To improve the situation we allow arbitrary variations on the boundary

$$\begin{aligned} \mathsf{d}F &= \int \frac{\delta F}{\delta \phi_A} \delta\phi_A \equiv \int_\Omega f'_A(\delta\phi_A) \equiv \\ &\equiv \int_\Omega D_J\left(E_A^J(f)\delta\phi_A\right), \end{aligned} \tag{10}$$

where the differential is written consequently by using the full variational derivative [14]

$$\frac{\delta F}{\delta \phi_A} = (-1)^{|J|} E_A^J(f) \theta_\Omega^{(J)} \equiv E_A^0(\theta_\Omega f), \tag{11}$$

the Frechét derivative

$$f'_A = \frac{\partial f}{\partial \phi_A^{(J)}} D_J, \tag{12}$$

and the higher Eulerian operators (6).

The second constituent, a Poisson bivector, is given, loosely speaking, by Poisson brackets of the fields. These brackets are called local if they are proportional to the δ-function and a finite number of its derivatives (ultralocal, if derivatives are absent)

$$\{\phi_A(x), \phi_B(y)\} = \hat{I}_{AB}(x)\delta(x, y), \tag{13}$$

where

$$\hat{I}_{AB}(x) = I_{AB}^L D_L, \qquad I_{AB}^L = I_{AB}^L(\phi_C^{(J)}). \tag{14}$$

The new feature of our formalism is that the surface contributions to this brackets are allowed [13]

$$\{\phi_A(x), \phi_B(y)\} = \theta_\Omega^{(K)}(x) \hat{I}_{AB}^{\langle K \rangle}(x)\delta(x, y). \tag{15}$$

For example, Ashtekar's transformation in the canonical gravity which is of the type (9) leads to the generalized form of the Poisson brackets given above [18]. This is a rather general feature of transformations of this type. We consider another example connected with the nonlinear Schrödinger equation in other place [19].

Even if the Poisson brackets of fields do not contain surface contributions such contributions may arise in the calculations of the Poisson algebras for some transformation generators constructed by means of these fields. It is so because these nonstandard terms may be a result of moving the derivatives of the δ-function from one of its arguments to another. The standard rule

$$\hat{I}_{AB}(x)\delta(x,y) = \hat{I}^{*}_{AB}(y)\delta(x,y), \tag{16}$$

is applicable but with the definition of the adjoint operator modified to preserve all the boundary terms

$$\begin{aligned} I^{*\langle J\rangle M}_{AB} &= (-1)^{|K|}\binom{K}{L}\binom{K-L}{M}\times \\ &\times \quad D_{K-L-M} I^{\langle J-L\rangle K}_{BA}. \end{aligned} \tag{17}$$

For example, if we preserve the boundary contributions, then the usual formula

$$\left(\frac{\partial}{\partial x^i} + \frac{\partial}{\partial y^i}\right)\delta(x,y) = 0, \tag{18}$$

should be replaced by the new one

$$\left(\theta_\Omega(x)\frac{\partial}{\partial x^i} + \theta_\Omega(y)\frac{\partial}{\partial y^i}\right)\delta(x,y) = -\theta^{(i)}_\Omega\delta(x,y).$$

This solves one paradox which arises in understanding the result obtained for asymptotically flat spaces in the canonical General Relativity. It is shown [7,8] that

$$\{H(\xi), H(\eta)\} \approx H([\xi,\eta]), \tag{19}$$

where ξ^α, η^β are the Killing vectors of the background flat metric, $[\xi,\eta]$ is their Lie bracket and $H(\xi)$, $H(\eta)$, $H([\xi,\eta])$ are generators with nonzero surface terms. The paradox is in the observation that if we first consider integrands of (19) and calculate their Poisson brackets according to (18) then we will get zero result due to the closed constraint algebra of the General Relativity.

The third step in our revision of the Poisson bracket formula is dictated by purely mathematical reasons. Speaking in mathematical terms, the extension of the formal variational calculus proposed above is the introduction of a new grading.

A grading in linear space L is a decomposition of it into a direct sum of subspaces, with a special value of some function p (grading function) assigned to all the elements of any subspace [6].

Here the function p takes its values in the set of all positive multi-indices and thus,

$$L = \bigoplus_{J=0}^{\infty} L^{\langle J\rangle}. \tag{20}$$

Elements of each subspace are called homogeneous.

A bilinear operation $x, y \mapsto x \circ y$, defined on L, is said to be compatible with the grading if the product of any homogeneous elements is also homogeneous, and if

$$p(x \circ y) = p(x) + p(y). \tag{21}$$

It is necessary to define the pairing between 1-forms and 1-vectors, which then really will induce all other operations, as an operation compatible with the introduced grading. In our notions 1-forms are

$$\alpha = \int \theta^{(J)}_\Omega \alpha^{\langle J\rangle}_{AK} D_K \delta\phi_A, \tag{22}$$

whereas 1-vectors are

$$\psi = \int \theta^{(I)}_\Omega \psi^{\langle I\rangle}_{BL} D_L\left(\frac{\delta}{\delta\phi_B}\right). \tag{23}$$

Their bases are dual

$$\left\langle \delta\phi_A(x), \frac{\delta}{\delta\phi_B(y)}\right\rangle = \delta_{AB}\delta(x,y), \tag{24}$$

and the graded differential operators

$$\hat{\alpha} = \theta^{(J)}_\Omega \alpha^{\langle J\rangle}_{AK} D_K, \tag{25}$$

$$\hat{\psi} = \theta^{(I)}_\Omega \psi^{\langle I\rangle}_{BL} D_L, \tag{26}$$

serve as coefficients of the decomposition over these bases. Let us define a trace as

$$\mathrm{Tr}(\hat{\alpha}\hat{\psi}) = \theta_\Omega^{(I+J)} D_L \alpha_{AK}^{\langle J\rangle} D_K \psi_{AL}^{\langle I\rangle}, \tag{27}$$

that is evidently a bilinear and commutative operation. It is also easy to check that

$$\mathrm{Tr}((D\hat{\alpha})\hat{\psi}) = D\mathrm{Tr}(\hat{\alpha}\hat{\psi}). \tag{28}$$

This important property of the trace operation allows us to use it for the definition of the pairing

$$\alpha(\psi) = \psi \,\lrcorner\, \alpha = \int \mathrm{Tr}(\hat{\alpha}\hat{\psi}), \tag{29}$$

which is independent on the ambiguity in the representations of the operators $\hat{\alpha}$, $\hat{\psi}$ following from the freedom to do the formal integration by parts. For example, we can remove all the derivatives from the basis elements

$$\alpha = \int \theta_\Omega^{(J)} \tilde{\alpha}_A^{\langle J\rangle} \delta\phi_A, \tag{30}$$

$$\psi = \int \theta_\Omega^{(I)} \tilde{\psi}_B^{\langle I\rangle} \frac{\delta}{\delta\phi_B}, \tag{31}$$

thus transforming α and ψ to the so-called canonical form (compare with [5]). This formal integration by parts does not change any integral over the finite domain Ω and is useful for the illustration of analogy with the standard formalism. To return back to the usual formal variational calculus we should only put $\theta_\Omega(x) \equiv 1$, i.e., $\Omega = \mathbb{R}^n$ then the "columns" like $\alpha^{\langle J\rangle}$ will be reduced to their first terms $\alpha^{\langle 0\rangle}$ and for the canonical representation of the 1-vector and 1-form their pairing will be reduced to the standard one

$$\psi \,\lrcorner\, \alpha = \int \tilde{\alpha}_A^{\langle 0\rangle} \tilde{\psi}_A^{\langle 0\rangle}. \tag{32}$$

After making the above three steps: the revision of differential, Poisson bivector and pairing we can obtain the new formula. There are at least three ways to write it, in correspondence to the three ways to write the differential of a local functional: through the full variational derivatives

$$\{F, G\} = \int\int \frac{\delta F}{\delta\phi_A(x)} \frac{\delta G}{\delta\phi_B(y)} \hat{I}_{AB}(x)\delta(x,y), \tag{33}$$

through the Frechét derivatives

$$\{F, G\} = \int \theta_\Omega^{(J)} \mathrm{Tr}\left(f'_A \hat{I}_{AB}^{\langle J\rangle} g'_B\right), \tag{34}$$

and through the higher Eulerian operators

$$\{F, G\} = \int \theta_\Omega^{(J)} D_{P+Q}\left(E_A^P(f) \hat{I}_{AB}^{\langle J\rangle} E_B^Q(g)\right). \tag{35}$$

3. EXAMPLES

The calculation of the Poisson brackets by the new formulas can be made in not more complicated way than by the old ones. First, to get the Frechét derivative from the first variation is even easier than to get the standard Euler-Lagrange derivative because the integration by parts is not needed. Second, we can exploit covariance properties and use the covariant derivatives instead of the ordinary ones.

As an example, we calculate the Poisson brackets of the two spatial diffeomorphism generators in the canonical General Relativity for a finite domain

$$\begin{aligned} H(N^i) &= \int_\Omega \pi^{ij}(\nabla_j N_i + \nabla_i N_j) d^3x = \\ &= \oint_{\partial\Omega} 2\pi_i^j N^i dS_j - \int_\Omega 2N^i \nabla_j \pi_i^j d^3x. \end{aligned} \tag{36}$$

From the first variation we get

$$\begin{aligned} h'_{\pi^{ij}}(N^i) &= \nabla_j N_i + \nabla_i N_j, \\ h'_{\gamma_{ij}}(N^i) &= \pi^{ik}\nabla_k N^j + \pi^{kj}\nabla_k N^i + N^k \pi^{ij} \nabla_k, \end{aligned} \tag{37}$$

and then calculate the Poisson bracket according to formula (34)

$$\{H(N^i), H(M^i)\} = H([N, M]^i), \tag{38}$$

where

$$[N, M]^i = N^k M^i{}_{,k} - M^k N^i{}_{,k}. \tag{39}$$

Let us mention that the calculation according to the standard formula gives additional surface contribution violating the diffeomorphism algebra

$$\begin{aligned} \Delta H &= \oint_{\partial\Omega} \pi^{ij}\left((\nabla_j N_i + \nabla_i N_j)M^k - \right. \\ &- \left. (\nabla_j M_i + \nabla_i M_j)N^k\right) dS_k. \end{aligned} \tag{40}$$

This violation is zero in the only case when N^i and M^i are the Killing vectors on the boundary. Therefore we have a free boundary closure of the spatial diffeomorphism algebra by means of the new brackets.

As a second example let us consider the Yang-Mills field in a finite domain. It is suitable to use orthonormal curvilinear coordinates X_k in $\mathbb{R}^3$, so that they are compatible with the boundary $\partial\Omega = \{X_k : X_1 = R = \text{const}, \breve{\mathbf{X}} = X_2, X_3\}$. If x_k are Cartesian coordinates then the local frame

$$e_i^{(k)} = h_k^{-1}\frac{\partial x_i}{\partial X_k}, \qquad h_k = \sqrt{\left(\frac{\partial x_i}{\partial X_k}\right)^2}, \tag{41}$$

can be used. The Hamiltonian has the form [20]

$$\begin{aligned} H_\Omega &= \int_\Omega d\mathbf{x}\left(\frac{1}{2}(E_i^a)^2 + \frac{1}{4}(F_{ij}^a)^2\right. \\ &- \left. A_0^a\left(\partial_i E_i^a - gt^{abc}A_i^b E_i^c\right)\right). \end{aligned} \tag{42}$$

It should be accompanied by the surface contribution

$$\Delta H_\Omega = \int_{\partial V} d\breve{\mathbf{X}}\; A_0^a\left(\frac{h}{h_1}E_{(1)}^a + \chi^a\right), \tag{43}$$

where $h = h_1 h_2 h_3$, and χ^a are the surface variables possessing the Poisson bracket

$$\{\chi^a(\breve{\mathbf{X}}), \chi^b(\breve{\mathbf{X}}')\} = gt^{abc}\,\chi^c(\breve{\mathbf{X}})\,\delta(\breve{\mathbf{X}}, \breve{\mathbf{X}}'), \tag{44}$$

and commuting with the volume variables. After fixing the spatial Fock-Schwinger gauge, $A_{(1)}^a = 0$, the Hamiltonian evolution on the boundary is given by

$$\begin{aligned} \dot{E}_{(1)}^a(R, \breve{\mathbf{X}}) &= -gt^{abc}E_{(1)}^b(R, \breve{\mathbf{X}})A_0^c(R, \breve{\mathbf{X}}), && (45) \\ \dot{\chi}^a(\breve{\mathbf{X}}) &= gt^{abc}\,\chi^b(\breve{\mathbf{X}})\,A_0^c(R, \breve{\mathbf{X}}), && (46) \end{aligned}$$

where the boundary condition $G_{(1)}^a(R, \breve{\mathbf{X}}) = 0$, $G_i^a \equiv \nabla_j F_{ij}^a$ compatible with the localized time evolution is also assumed.

Here the Gauss law constraint is prolonged onto the boundary by introduction of the surface variables $\chi^a(\breve{\mathbf{X}})$. The standard approach requires a fixation of the static boundary conditions for $E_{(1)}^a$, and in its turn this requires that the Lagrangian multiplier A_0^c should be zero on the boundary. Then the boundary conditions are to be gauge-dependent or $E_{(1)}^a$ be zero. The approach based on the dynamical boundary conditions permits to save gauge invariance on the boundary.

The residual gauge invariance of the theory is manifested in the above dynamics on the boundary. This implies that the boundary conditions put onto $E_{(1)}^a$ may not necessarily be arbitrary to preserve the gauge invariance. It has been argued that the dependence of the partition function on these boundary conditions may be considered as a confinement criterion in the SU(N) gauge theory [23], and that the surface terms play an important role for understanding that phenomenon [22].

4. CONCLUSION

As we have seen from above, the Poisson structure can be introduced prior to any boundary conditions. This is analogous to the Hamiltonian mechanics where constraints are treated later than the Poisson brackets. We may expect that the treatment of the boundary conditions could proceed similarly, so that primary and secondary, first and second class boundary conditions may arise. We may get an analog of the Dirac bracket at the end of the standard reduction procedure.

What are the Hamiltonian equations generated by the new bracket? They can be called as a weak form of the equations of motion [2]. If we try to understand θ_Ω-functions as distributions seriously, then we will have singular boundary terms in the equations and may encounter with ambiguities in solving such equations. Therefore, the construction of the closed Poisson algebras with surface terms seems to be a more promising direction. There we deal with local functionals, rather than functions, and the Poisson bracket does not move us out of that class. It is quite possible that the Hamiltonian dynamics for the functionals may become of more importance for the quantum field theory than for the classical one.

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